

# Superconductivity on the density wave background with soliton-wall structure

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## Abstract

Superconductivity (SC) may microscopically coexist with density wave (DW) when the nesting of the Fermi surface (FS) is not perfect. There are, at least, two possible microscopic structures of a DW state with quasi-particle states remaining on the Fermi level and leading to the Cooper instability: (i) the soliton-wall phase and (ii) the small ungapped Fermi-surface pockets. The dispersion of such quasi-particle states strongly differs from that without DW, and so do the properties of SC on the DW background. The upper critical field  $H_{c2}$  in such a SC state strongly increases as the system approaches the critical pressure, where superconductivity first appears.  $H_{c2}$  may considerably exceed its typical value without DW and has unusual upward curvature as function of temperature. The results obtained explain the experimental observations in layered organic superconductors (TMTSF)<sub>2</sub>PF<sub>6</sub> and  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub>.

*Key words:* spin density wave, CDW, superconductivity, quantum critical point, upper critical field, solitons

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## 1. Introduction

The interplay of superconductivity (SC) and density-wave (DW) states appears in many compounds and is extensively investigated for several decades (see, e.g., reviews in Refs. [1],[2]). The DW removes electrons from the Fermi level, and, usually, precludes superconductivity[3] or strongly reduces the SC transition temperature[4]. However, in several compounds [e.g., in layered organic superconductors (TMTSF)<sub>2</sub>PF<sub>6</sub> and  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub>],[5, 6] the SC transition temperature  $T_c^{SC}$  on the DW background is very close to (or even exceeds)  $T_c^{SC}$  without DW. In both these compounds SC coexists with DW in some pressure interval  $P_{c1} < P < P_c$ : superconductivity first appears at  $P = P_{c1}$ , and at  $P_c$  the DW phase undergoes a phase transition into the metallic state (see Fig. 7 in Ref. [5] and the schematic phase diagram in Fig. 1). In this region SC state has many unusual properties, such as the divergence of the upper critical field  $H_{c2}$  at  $P \rightarrow P_{c1}$ . [7, 6] To explain this property, the scenario of macroscopic spatial separation of SC and DW states was proposed, where the size  $d_s$  of SC domains depends on magnetic field and in strong magnetic field becomes much smaller than the SC coherence length  $\xi_{SC}$ . [7] When the width  $d_s$  of a type II superconducting slab becomes smaller than  $\xi_{SC}$ , the upper critical field  $H_{c2}$  is increased compared to  $H_{c2}^0$  in

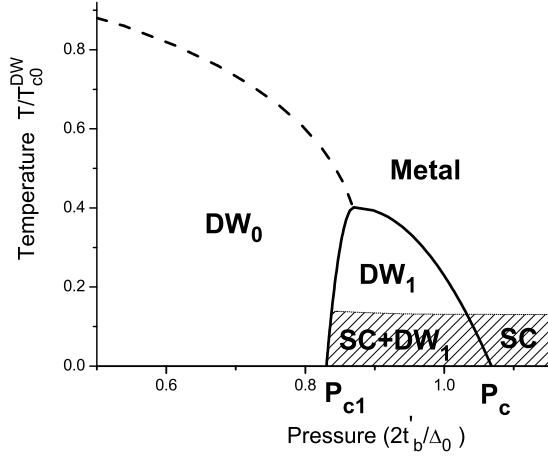


Figure 1: The schematic picture of the phase diagram in  $(\text{TMTSF})_2\text{PF}_6$ , where superconductivity coexists with DW in some pressure interval above  $P_{c1}$  but below  $P_c$ .  $\text{DW}_0$  stands for the uniform fully gapped DW.  $\text{DW}_1$  denotes the DW state when the imperfect nesting term  $2t'_b > \Delta_0$ , so that the ungapped FS pockets or nonuniform DW structure appear.

a bulk superconductor by a factor (see Eq. 12.4 of Ref. [8])

$$H_{c2}/H_{c2}^0 \approx \sqrt{12}\xi_{SC}/d_s. \quad (1)$$

For  $(\text{TMTSF})_2\text{PF}_6$  and for many other DW superconductors this scenario implies the size of the SC domains to be of the order of the DW coherence length  $\xi_{DW}$ , which means a strong influence of the DW order parameter on the SC properties and a microscopic coexistence of these two states. Such a strong spatial modulation of the DW order parameter costs energy  $W$  of the order of the DW energy gap  $\Delta_0$ , which is much larger than the energy gain due to the surviving of SC state. In this case, the soliton wall scenario[9, 10, 11, 12, 13, 14] is more favorable, where the energy loss  $W$  due to nonuniform DW order parameter is compensated by the large kinetic energy of soliton-band quasiparticles.[11, 13] SC appearing in the soliton wall phase of spin-density wave (SDW) has the triplet SC pairing[14] in agreement with experiments in  $(\text{TMTSF})_2\text{PF}_6$ . [15] Another microscopic structure was proposed[14] and investigated[16] recently, where the small ungapped Fermi-surface pockets in the DW state appear due to the imperfect nesting of Fermi surface (FS) and lead to the SC instability. In that scenario the divergence of upper critical field  $H_{c2}$  at  $P \rightarrow P_{c1}$  is due to the decrease of the mean square velocity on the Fermi surface when the size of the new FS pockets decreases.[16] In the present paper, we continue to study the SC properties on the DW background. We calculate  $H_{c2}$  in the soliton-wall scenario and show how the divergence of  $H_{c2}$  at  $P \rightarrow P_{c1}$  appears on the soliton-phase background. Within this scenario we also explain the upward curvature of the temperature dependence of  $H_{c2z}$  along the  $z$ -axis perpendicular to the conducting layers. The possibility to explain the same feature within the open-pocket scenario and the limitations of the weak-coupling theory to describe this effect are briefly discussed. We also explain the observed hysteresis in the pressure dependence of SC transition temperature  $T_c^{SC}(P)$  in both above scenarios.

## 2. The model and the DW state without superconductivity

Below we consider the same model, as in Ref. [14]. The quasi-1D free electron dispersion without magnetic field has the form

$$\varepsilon(\mathbf{k}) = \pm v_F(k_x \mp k_F) + t_\perp(\mathbf{k}_\perp), \quad (2)$$

where the interchain dispersion  $t_\perp(\mathbf{k}_\perp)$  is much weaker than the in-plane Fermi energy  $v_F k_F$  and given by the tight-binding model with few leading terms:

$$t_\perp(\mathbf{k}_\perp) = 2t_b \cos(k_y b) + 2t'_b \cos(2k_y b). \quad (3)$$

Here  $b$  is the lattice constants in the  $y$ -direction. The dispersion along the  $z$ -axis is considerably weaker than along the  $y$ -direction and is omitted. The FS consists of two warped sheets and possesses an approximate nesting property,  $\varepsilon(\mathbf{k}) \approx -\varepsilon(\mathbf{k} - \mathbf{Q}_N)$ , with  $\mathbf{Q}_N$  being the nesting vector. The nesting property leads to the formation of DW at low temperature and is only spoiled by the second term  $t'_b(k_y)$  in Eq. (3), which, therefore, is called the "antinesting" term. Increase of the latter with applied pressure leads to the transition in the DW<sub>1</sub> state at  $P > P_{c1}$ , where the quasi-particle states on the Fermi level first appear and lead to the SC instability. In the pressure interval  $P_{c1} < P < P_c$  the new state develops, where the DW coexists with superconductivity at rather low temperature  $T < T_c^{SC}$ , while at higher temperature  $T_{SC} < T < T_{DW}$  the DW state coexists with the metallic phase. This coexistence takes place via the formation of small ungapped pockets[16] or via the soliton phase[12, 13, 14]. We take the DW transition temperature to be much greater than the SC transition temperature,  $T_c^{DW} \gg T_c^{SC}$ , which corresponds to most DW superconductors. For example, in (TMTSF)<sub>2</sub>PF<sub>6</sub>  $T_c^{DW} \approx 8.5K \gg T_c^{SC} \approx 1.1K$ , and in  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub>,  $T_c^{DW} \approx 8K \gg T_c^{SC} \approx 0.1K$ . Therefore, we first study the structure of the DW state in the pressure interval  $P_{c1} < P < P_c$ , and then consider the superconductivity on this background.

In the soliton phase, which presumably establishes in the pressure interval  $P_{c1} < P < P_c$ , the DW order parameter depends on the coordinate along the conducting chains:  $\Delta(x) \approx \Delta_0 \text{sn}(x/\xi_{DW})$ , where  $\text{sn}(y)$  is the elliptic sinus function. As a result an array of soliton walls of width  $\xi_{DW}$  get formed, where the DW order parameter changes sign. Each soliton wall contributes one electron-like quasiparticle per conducting chain on the Fermi level, which leads to the formation of the new conducting soliton band. This soliton band appears in the middle of the DW energy gap and has the dispersion

$$E(\mathbf{k}) = E(k_x) + \varepsilon_+(k_y), \quad (4)$$

where the interchain part of the dispersion is given by the antinesting term in the dispersion (3):  $\varepsilon_+(\mathbf{k}_\perp) = [t_\perp(\mathbf{k}_\perp) + t_\perp(\mathbf{k}_\perp - \mathbf{Q}_\perp)]/2$ . The dispersion  $E(k_x)$  along the conducting chains was found in Ref. [19] (see Fig. 1 in Ref. [19]), and for qualitative analysis it can be approximated by

$$E(k_x) \approx E_- \sin[\pi(|k_x| - k_F)/2\kappa_0]. \quad (5)$$

The soliton band width  $E_-$  and boundary  $\kappa_0$  in the momentum space are determined by the linear concentration  $n_s$  of the soliton walls[19]:  $\kappa_0 = \pi n_s/2$ ,  $\hbar v_F n_s = E_+/K \left( \sqrt{1 - E_-^2/E_+^2} \right)$ ,

where  $K(r)$  is the complete elliptic integral of the 1st kind. At  $n_s \rightarrow 0$   $E_+ \approx \Delta_0$ , and  $E_- \approx 4\Delta_0 \exp(-\Delta_0/\hbar v_F n_s)$ . Note, that the soliton phase can be energetically most favorable DW state at imperfect nesting.[13] Compared to the uniformly gapped DW state, the soliton phase gains the kinetic energy of quasiparticles in the half-filled soliton phase due to the term  $\varepsilon_+(k_y)$  in (4), which compensates the energy loss of the non-uniform DW structure.

The soliton wall concentration  $n_s$  depends on external pressure  $P$  via the dependence on electron dispersion.  $n_s(P)$  can be obtained by minimization of the total energy of the soliton phase (see Eqs. (33)-(35) of Ref. [11] or Eqs. (9)-(12) of Ref. [13]). The result substantially depends on the harmonic content of electron dispersion  $t_\perp(\mathbf{k}_\perp)$ [13]. For typical dispersion, at  $P \rightarrow P_{c1}$  the soliton band width  $E_-/\Delta_0 \rightarrow 0$ , which corresponds to a phase transition from the uniform DW to the soliton phase. In the vicinity of  $P = P_{c1}$ , rough estimates give[17]

$$E_- \sim \sqrt{\Delta_0 \delta} \equiv \sqrt{\Delta_0 (2t'_b - \Delta_0)} \propto \sqrt{P - P_{c1}}. \quad (6)$$

### 3. SC properties on the soliton-phase DW background

In the Ginzburg-Landau functional for SC state the coefficient tensor  $1/m_{ij}$  before the gradient term can be expressed via the product  $\langle v_i v_j \rangle$  of electron velocities  $v_i$  averaged over the Fermi surface[20] [see Eqs. (48)-(50) of Ref. [16]. Using this result and the simplified dispersion (4),(5) in the soliton band one easily obtains

$$\begin{aligned} \frac{1}{m_{yy}} &= \frac{14\zeta(3)(t'_b b)^2}{3\pi^2 T_c^{SC} \hbar^2}, \\ \frac{1}{m_{xx}} &= \frac{7\zeta(3)E_-^2(\pi/2\kappa_0)^2}{24\pi^2 T_c^{SC} \hbar^2} = \frac{7\zeta(3)E_-^2}{24\pi^2 T_c^{SC} \hbar^2 n_s^2}, \end{aligned} \quad (7)$$

and the upper critical field  $H_{c2}^z = (c/e\hbar)(T_c^{SC} - T)\sqrt{m_{xx}m_{yy}}$  along the z-axis is

$$H_{c2}^z = C_{1s} \frac{T_c^{SC}(n_s \xi_{SDW})}{E_-} \frac{c(T_c^{SC} - T)}{ebv_F}, \quad (8)$$

where  $\xi_{DW} = \hbar v_F/\pi\Delta_0$ ,  $n_s \xi_{DW} \approx 1/\pi \ln(4\sqrt{2}\Delta_0/E_-)$ , and the constant  $C_{1s} = 12\pi^3/7\zeta(3) \approx 44.2$ . Eq. (8) is similar to Eq. (55) of Ref. [16] for the second scenario, where the open pocket size  $\delta = 2t'_b - \Delta_0$  is replaced by the soliton band width  $E_-$ . At  $P \rightarrow P_{c1}$  both  $\delta \rightarrow 0$  and  $E_- \rightarrow 0$ , and in both scenarios the functions  $\delta(P)$  and  $E_-(P)$  depend on the electron dispersion  $t_\perp(\mathbf{k}_\perp)$ . Substituting (6) into (8), one obtains that in the soliton-wall scenario the slope  $dH_{c2}^z/dT \propto 1/\sqrt{P - P_{c1}}$  and the upper critical field  $H_{c2}$  diverge at  $P \rightarrow P_{c1}$  similar to the scenario of the ungapped FS pockets[16]. The physical reason for this divergence is the strong change of quasi-particle dispersion on the Fermi level when  $P \rightarrow P_{c1}$  and the soliton band shrinks. This shrinking leads to the decrease in the mean square electron velocity on the Fermi level (or diffusion coefficient), which increases the upper critical field  $H_{c2}$ .

For (TMTSF)<sub>2</sub>PF<sub>6</sub> the substitution of  $E_- \sim \sqrt{\Delta_0 \delta}$  to (8) gives the slope

$$\frac{dH_{c2}^z}{dT} \approx \frac{7.8}{\ln(4\sqrt{2}\Delta_0/\delta)} \frac{T_c^{SC}}{\sqrt{\Delta_0 \delta}} \left[ \frac{\text{Tesla}}{^\circ K} \right]. \quad (9)$$

and the maximum slope  $dH_{c2}^z/dT \approx 0.6 [Tesla/^{\circ}K]$  in a reasonable agreement with the experiment (see Fig. 2 in Ref. [7]). Far from  $P = P_{c1}$ ,  $E_- \approx \Delta_0$ , and Eq. (8) gives  $dH_{c2}^z/dT \approx 0.25 [Tesla/^{\circ}K]$ , which is again in a good agreement with experimental data in Fig. 2 of Ref. [7]. For  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub>, the substitution of  $E_- \approx \Delta_0$  to (8), using BCS relation  $\Delta_0 = 1.76T_c^{CDW}$ , gives  $H_{c2}^z \approx 7.7 \text{ mTesla} \cdot (1 - T/T_c^{SC})$ , or  $dH_{c2}^z/dT \approx 77 [mTesla/^{\circ}K]$  in a qualitative agreement with experiment[6].

The upward curvature of  $H_{c2}^z(T)$  in the scenario of soliton walls is similar to  $H_{c2}(T)$  in layered superconductors when magnetic field is parallel to the conducting layers. The latter case was considered in a number of theoretical papers (see, e.g., [21],[22],[23], or §16 of [8]). The 1D network of soliton walls can be considered as a 1D Josephson lattice, where the conducting layers of thickness  $\xi_{DW}$  are separated by the insulating layers by thickness  $s = 1/n_s$ . At low field this Josephson lattice behaves like a 3D superconductor with critical field  $H_{c2}^i = e_{ijk}\Phi_0/2\pi\xi_j(T)\xi_k(T)$ , where  $\Phi_0$  is magnetic flux quantum and  $\xi_i(T)$  is the SC correlation length in  $i$ -direction. In the vicinity of critical temperature  $\xi_i \propto (T_{cSC} - T)^{-1/2}$ . At high field  $H_{c2}$  tends to its value (1) in the 2D SC slab of thickness  $d_s \sim \xi_{DW} \ll \xi_{SC}$ . [23] For (TMTSF)<sub>2</sub>PF<sub>6</sub>,  $\xi_{DW}/\xi_{SC} \approx 1/10$ , and according to Eq. (1), the upper critical field  $H_{c2}^z$  on the SDW background can be enhanced by a factor  $H_{c2}/H_{c2}^0 \lesssim 30$  as compared to  $H_{c2}^{z0}$  in the bulk superconductor, i.e. superconductor without the soliton structure.

The crossover from the 3D to 2D behavior of  $H_{c2}^z$  occurs when the soliton bandwidth becomes small:  $E_- < \hbar^2/m_y\xi_{SC}^2$ , where  $\xi_{SC} \approx \hbar v_{y\max}/\pi\Delta_{SC}(T)$  is the temperature dependent correlation length within the conducting layer, and  $m_y \approx t'_b/v_{y\max}^2$ . This gives the crossover value  $E_- \sim [\pi\Delta_{SC}(T)]^2/t'_b$ . Therefore, the upper critical field increases and behaves as in the isolated SC slab only at  $P \rightarrow P_{c1}$  and only at low temperature, which means the unusual upward curvature of  $H_{c2}^z(T)$  at  $P \rightarrow P_{c1}$ . Note, that the soliton structure is important for the upward curvature of only z-component  $H_{c2}^z(T)$  of magnetic field in layered organic metals as (TMTSF)<sub>2</sub>PF<sub>6</sub> or  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub>, because it creates the layered soliton wall structure parallel to the magnetic field. If magnetic field lies in the x-y plane, it is already parallel to the conducting molecular layers, and  $H_{c2}^z(T)$  may have the upward curvature according to the Lawrence-Doniach model even without soliton walls.

#### 4. Discussion and summary

The above study gives a rough estimates of the upper critical field  $H_{c2}(P, T)$  in the soliton phase. The divergence and the unusual upward curvature of  $H_{c2}^z(T)$  at  $P \rightarrow P_{c1}$ , observed in (TMTSF)<sub>2</sub>PF<sub>6</sub> and  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub>, are explained. A quantitative study of  $H_{c2}(P, T)$  requires a more accurate model for the coexisting SC and DW states, which includes the influence of SC on the DW state. The critical fluctuations near the DW-metal phase transition also strongly influence the SC state via the renormalization of the e-e interaction.[1, 24, 25] However, the proposed rough model gives a reasonable quantitative agreement with experiment on the slope of  $H_{c2}^z(T)$  at  $T \rightarrow T_c^{SC}$ .

One more unusual feature observed in these compounds is the hysteresis in the pressure dependence of the SC transition temperature  $T_c^{SC}(P)$ . In the soliton scenario this hysteresis may come from the motion of soliton walls in order to achieve the optimal soliton-wall concentration  $n_s(P)$  as pressure  $P$  changes. The hysteresis in  $T_c^{SC}(P)$  can also be explained in the open-pocket scenario if the DW wave vector shifts at  $P > P_{c1}$  with change in pressure

to find the optimal DW wave vector at imperfect nesting. Since the DW wave vector is pinned by crystal imperfections, this shift of the DW wave vector is hysteretic, which leads to the hysteresis in  $\delta$  and in the SC transition temperature  $T_{SC}$ .

An accurate description of the SC properties in both scenarios must go beyond the weak-coupling theory, because the new Fermi energy (i.e.,  $\delta$  in the new FS pockets or the bandwidth  $E_-$  in the soliton phase) is comparable to the SC energy gap as  $P \rightarrow P_{c1}$  and is much smaller than the Debye energy. This fact, for example, may be responsible for the upward curvature of  $H_{c2}^z(T)$  in the scenario of open pockets, where

$$H_{c2}^z \propto 1/\sqrt{\langle v_x^2 \rangle \langle v_y^2 \rangle} \propto 1/\delta. \quad (10)$$

When  $\delta < T_c^{SC}$ , the small value of  $\delta$  is smeared out by high temperature. Qualitatively, this smearing may be included via the replacement  $\delta \rightarrow \sqrt{\delta_0^2 + \alpha T^2}$ ,  $\alpha \sim 1$ . At  $P \rightarrow P_{c1}$  substituting this and  $\delta_0 \propto P - P_{c1}$  to (10), one obtains

$$H_{c2}^z \propto 1/\sqrt{\beta (P - P_{c1})^2 + \alpha T^2}, \quad (11)$$

which gives the upward curvature of  $H_{c2}^z(T)$  and describes well the experimental data in Ref. [7] with two fitting parameters  $\alpha$  and  $\beta$ .

The proposed approximate model of the SC state on the soliton-wall background of the DW at  $P > P_{c1}$  qualitatively explains all unusual SC properties on the DW background observed in the organic metals (TMTSF)<sub>2</sub>PF<sub>6</sub> and  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub>, which gives a strong argument in favour of the microscopic coexistence of superconductivity and density-wave state in these compounds.

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